

Isophthalic acid, isobutyl tridec-2-ynyl ester

Inchi: InChI=1S/C25H36O4/c1-4-5-6-7-8-9-10-11-12-13-14-18-28-24(26)22-16-15-17-23(19-22)
InchiKey: HIAUMVMETFPUSA-UHFFFAOYSA-N
Formula: C25H36O4
SMILES: CCCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-5.08	kJ/mol	Joback Method
hf	-556.85	kJ/mol	Joback Method
hfus	59.33	kJ/mol	Joback Method
hvap	94.26	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.190		Crippen Method
mvol	345.630	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	3026.00		NIST Webbook
rinpol	3026.00		NIST Webbook
tb	964.20	K	Joback Method
tc	1182.87	K	Joback Method
tf	645.87	K	Joback Method
vc	1.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.14	J/molxK	964.20	Joback Method
cpg	1142.26	J/molxK	1000.65	Joback Method
cpg	1156.95	J/molxK	1037.09	Joback Method
cpg	1170.25	J/molxK	1073.54	Joback Method
cpg	1182.20	J/molxK	1109.98	Joback Method
cpg	1192.84	J/molxK	1146.43	Joback Method
cpg	1202.21	J/molxK	1182.87	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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